

Growth of a One Dimensional Quasiperiodic Covering with Locally Determined Decorations.

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A growth mechanism for a perfect one-dimensional (1D) quasiperiodic structure is presented with a local covering rule. We use rectangular tiles with two different types of string decorations. The string position in a tile is allowed to move when the tile is attached to an existing patch. By adjusting the position properly with local information, we show that a growth of perfect quasiperiodic structure is possible. This observation may provide new insight into how quasicrystals grow with perfect quasiperiodic order.

How can quasicrystals grow with quasiperiodic order? This has been a fundamental question in the quasicrystal community from the discovery of quasicrystals [1]. Most quasicrystalline phases are observed in metallic alloys whose atomic interactions are believed to be short-ranged while the quasiperiodic arrangement seemingly requires non-local information.

The debates on the possibility of a local growth algorithm for a perfect quasicrystalline structure were fueled in a quite early stage of quasicrystal studies [2, 3, 4, 5, 6]. The discovery of thermodynamically stable quasicrystalline phases [7, 8, 9] showed the existence of genuine quasicrystals, but the deepest question on the physical origin of the non-crystallographic order has not been fully solved yet. The various viewpoints on the explanation fall into two paradigms: energy-driven perfect quasiperiodic quasicrystals and entropy-driven random-tiling quasicrystals. This energy-entropy debate has mainly focused on the origin of stability, but the same arguments can be applied to the growth of quasicrystals. Hence, we can imagine two alternative scenarios for quasicrystal growth; matching-rule based, energy-driven growth [2] and finite-temperature entropy-driven growth [6]. A major criticism for the former scenario is that non-local information is likely needed for a perfect quasiperiodic structure growth. Such criticisms were mainly based on Penrose's observation that no local growth rules can produce a perfect quasicrystalline tiling in two-dimensional (2D) space [5, 10]. Recently, we provided a local growth algorithm to produce a perfect quasicrystalline structure in 3D and showed that non-local information is not necessary for growth with the perfect quasiperiodic order [11]. However, the algorithm has an artificial element and works only with a special type of seed. Also, it can produce only one particular type of Penrose tiling known as the cartwheel tiling [12].

In this letter, we introduce a new type of local growth algorithm and show that perfect quasiperiodic structures can be grown with a local process even in 1D systems. Our growth rule is local in the sense that it determines

the type of attaching tile according to the decoration (information) of the tile to which the tile is attached. However, it is different from conventional growth rules in a couple of aspects. First, we use the covering and allow overlaps between neighboring tiles. Second, the position of decoration is not fixed prior to the attachment. We choose the decoration position when we attach the tile to the existing patch of tiles. The latter may not be a typical way of decoration for a matching rule in conventional tilings but seems to be physically plausible for the covering process. Physically, a tile usually represents a stable cluster atoms, but the positions of atoms can be adjusted a bit when it overlaps with neighboring clusters.

One can easily see that non-local information is needed for the growth of a 1D perfect quasiperiodic structure with a conventional growth rule in which decorations for the matching rule, as well as the shapes of the tiles, are fixed. Figure 1(a) shows a Fibonacci lattice, one of the most well known 1D quasiperiodic system and its "inflations". A Fibonacci lattice is a special 1D infinite arrangement of two types of tiles, say, A and B , which allows an infinite sequence of inflations, a composition $AB \rightarrow A$ and $A \rightarrow B$ shown in Fig. 1. To allow an inflation, a Fibonacci lattice should be decomposed as an infinite array of AB and A segments. In other words, there should not be BB segments in any part of a Fibonacci lattice. Furthermore, the inflation of a Fibonacci lattice should be another (infinite) Fibonacci lattice because it allows infinite iterative inflations. This requirement excludes AAA segments, which would produce BB segments after an inflation. By the same token, an $ABABAB$ segment is not allowed because its inflation would produce an AAA segment whose (next) inflation becomes a BB segment. The longer segments must be investigated to exclude the "forbidden" BB segments in the more inflated lattices. Hence, in order to grow a Fibonacci lattice, we need a non-local growth rule, which provides information on an increasing range of tile arrangement as the patch grows, as illustrated in Figs. 1(b) and (c).

Consider a growth from a "correct" (subset of a Fibonacci lattice) finite patch shown in the upper part of Fig. 1(b). When a tile is attaching to site v , its type is determined by one or two nearest sites. If a B -tile

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the relationship between coverings and tilings is trivial. We can always construct a covering corresponding to a given tiling by enlarging the basic building units. The mapping can be reversed to produce a tiling from a covering, reducing the basic building units until the units join edge-to-edge (point-to-point in pure 1D system) without overlap. Although the lattice structures of the covering and the tiling are equivalent, we use covering here because our adjustable decoration is more naturally expressed in terms of covering.

Figure 2 shows the basic building units and our growth rule. We use a rectangle tile with the size of $(1 + 2w) \times \tau$ as the basic building unit. Here, $\tau = (1 + \sqrt{5})/2$ is the golden mean, and $w > 0$ is an arbitrary positive number. In the figure, we choose $w = \frac{1}{2\tau}$ so that the unit becomes a square. There are two types of decorations, deco-A and deco-B, as shown in Fig. 2(a). Both decorations consist of three line segments, α , β , and γ . The segments α and γ are horizontal lines with lengths of w for both decorations, but the segments β have different slopes. For deco-A, the slope is $\beta_A = -1/\tau$ while for deco-B, it is $\beta_B = 1$. Their vertical positions are movable in the bounded regions denoted by the hatched lines of purple and skyblue. The vertical coordinate y_L of the segment α should satisfy $y_L \in \mathbb{D}_A^\alpha = [1/\tau, \tau)$ for deco-A while that of deco-B is given by $y_L \in \mathbb{D}_B^\alpha = [0, 1/\tau)$ so that their γ -segments remain in the tiles ($y_R = y_L - 1/\tau \geq 0$ for deco-A and $y_R = y_L + 1 < \tau$ for deco-B). In the growth process, a tile is added to an existing patch only if the string of the tile can adjust its vertical position so that its string decoration coincides with that of the existing patch in the overlapped region. This excludes BB arrangement and permits three ways of pairwise overlaps, AA , AB , and BA arrangements, for the isolated two tile configurations, as shown in Fig. 2(b). Both an A -tile (tile with deco A) and a B -tile (tile with deco B) can be added to an A -tile [15], but only an A -tile can be added to a B -tile because the γ -region of deco-B does not overlap with the α -region of deco-B. As the patch grows, the position of the string decoration at the boundary effectively carries the information on all tiles in the patch and forces the correct type of tile to be added. Figure 2(c) illustrates how our overlap rule excludes an incorrect configuration such as AAA or $ABABAB$. For an AA arrangement, y_R of the right A -tile is always smaller than $\tau - 2/\tau = 1/\tau^2$ while y_L of an A -tile cannot be smaller than $1/\tau$. If we attach an A -tile and move the string to the required position, it goes out of the tile, as shown by the dotted line in Fig. 2(c). When one type of tile is excluded, the other type of tile is always allowed because the α -regions of an A -tile and those of a B -tile are complementary to each other ($\mathbb{D}_A^\alpha \cup \mathbb{D}_B^\alpha = [1/\tau, \tau)$ and $\mathbb{D}_A^\alpha \cap \mathbb{D}_B^\alpha = \emptyset$). Therefore, a B -tile is forced to attach to an AA arrangement. Similar argument shows that an A -tile is forced to an $ABABA$ arrangement. As illustrated in the lower panel of Fig. 2(c), the γ -segment position of the rightmost A -tile y_R cannot be smaller than $2 - 2/\tau = 2/\tau^2$, which is larger than the maximum y_L value of a B -tile, $1/\tau$.

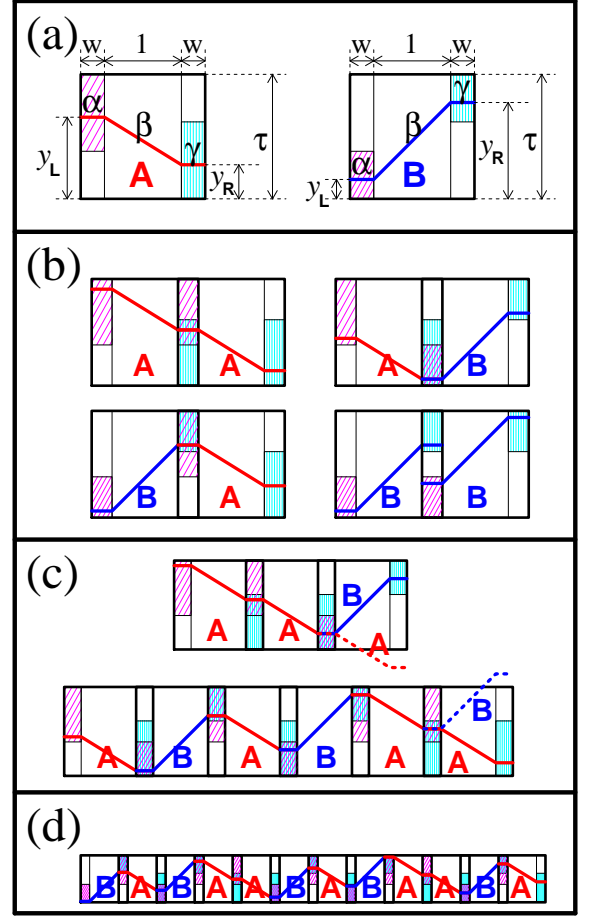


FIG. 2: (Color online) (a) Basic building units for the covering with two types of decorations, deco-A and deco-B. Each tile is a $(1 + 2w) \times \tau$ rectangle, and its decoration consists of three line segments, α , β , and γ . The slopes of the β -segments depend on the decoration types and are given by $\beta_A = -1/\tau$ and $\beta_B = 1$ for A and B types respectively. The vertical position of the string decoration is movable in the bounded regions. The vertical coordinate y_L of the α segments should satisfy $y_L \in [1/\tau, \tau)$ for deco-A and $y_L \in [0, 1/\tau)$ for deco-B so that the segment γ remains in the tile ($y_R = y_L - 1/\tau \geq 0$ for deco-A and $y_R = y_L + 1 < \tau$ for deco-B). (b) Overlap rule for the Fibonacci covering. Two neighboring rectangles in a covering overlap in the W -region. A rectangle can be overlapped with its neighbor only if the string of the rectangle can adjust its vertical position so that its string decoration coincides with that of the neighboring rectangle in the W -region. This excludes a BB arrangement and permits three pairwise overlaps, AA , AB , and BA arrangement, for the isolated two-tile configurations. (c) Growth of a Fibonacci covering. The overlap rule excludes incorrect configurations, such as AAA or $ABABAB$ arrangement (denoted by dotted lines), by allowing only a B -tile to an AA segment and an A -tile to an $ABABA$ segment. (d) Fibonacci covering corresponding to Fig. 1(a) with string decorations. String decorations can remain inside the rectangles when they are arranged as a Fibonacci lattice.

We have illustrated how our overlap rules exclude the

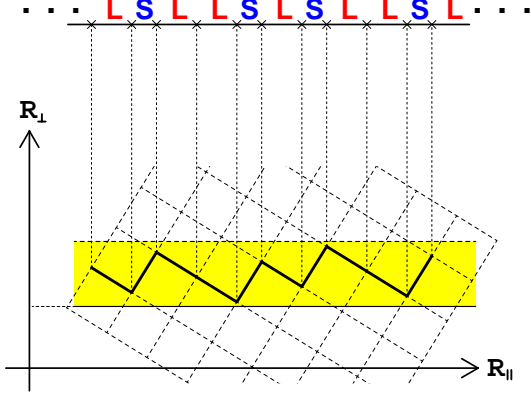


FIG. 3: (Color online) The lifting of a (pure 1D) Fibonacci lattice into a 2D hyper-space. A Fibonacci tiling consist of two types of tiles, say L and S , can be lifted into a 2D square lattice whose x -axis has the slope $-1/\tau$ with respect to the 1D tiling on \mathbb{R}_{\parallel} by mapping L to a x -edge and S to a y -edge of a square. The lengths of tiles L and S are given by $\cos\theta$ and $\sin\theta$, respectively, where $\tan\theta = 1/\tau$. The embedded step (solid thick line) in the 2D lattice can be covered by a strip parallel to \mathbb{R}_{\parallel} with width $\Delta = \cos\theta + \sin\theta$ when the position of the strip is well chosen. The \mathbb{R}_{\perp} coordinates of the step decrease by $\sin\theta$ for an L -tile and increase by $\cos\theta$ for an S -tile.

incorrect arrangement of tiles. Now, we see that our string decoration is possible for any correct configuration of Fibonacci lattice. In Fig. 2(d), string decorations are shown for the Fibonacci covering corresponding to Fig. 1(a). They coincide in all overlapped regions and remain in the unit cells.

We can show that Fibonacci lattices are grown by our local rule by lifting the covering to a 2D hyperspace. Any 1D tiling consisting of two types of tiles, say an L -tile and an S -tile, can be lifted into a “representative surface”, a step (denoted by solid thick line in Fig. 3) on a 2D square lattice by mapping one type to an x -edge and the other type to a y -edge of a square in the 2D space. Let us first consider a pure 1D Fibonacci tiling with (pure 1D) tiles whose lengths are given by $\cos\theta$ and $\sin\theta$ for tiles L and S , respectively, where $\theta = \arctan(1/\tau)$, as shown in Fig. 3. Then, we see that the \mathbb{R}_{\perp} coordinates of a representative surface (the step) in the hyper-space decreases by $\sin\theta$ for an L -tile and increases by $\cos\theta$ for an S -tile. Using this, we can calculate the \mathbb{R}_{\perp} coordinate changes for all series of inflated tiles and show that the embedded step in the 2D hyper-space can be covered by a strip parallel to \mathbb{R}_{\parallel} with width $\Delta = \cos\theta + \sin\theta$ when the position of the strip is well chosen [16, 17]. We can also show the converse, a 1D tiling whose embedded step is covered by the strip (with the \mathbb{R}_{\perp} width of Δ), is a Fibonacci tiling, by considering the mapping of the strip under inflation [16, 18]. Now, we need to show that the string decoration of our covering can be mapped to the embed-

ded step in the hyper space and that our growth rule, indeed, forces the step to be in a strip of proper width. Note that the overall length scale in the \mathbb{R}_{\perp} space is irrelevant as long as the ratio of the \mathbb{R}_{\perp} space coordinates of the two tile, $r = \Delta\mathbb{R}_{\perp}(L)/\Delta\mathbb{R}_{\perp}(S) = -1/\tau$, is fixed. If both $\Delta\mathbb{R}_{\perp}(L)$ and $\Delta\mathbb{R}_{\perp}(S)$ are increased by a factor of λ , then we can still get the Fibonacci lattice by simply increasing the strip width by the same factor. For numerical simplicity, we choose $\Delta\mathbb{R}_{\perp} = |y_R - y_L|$ of A -tile and B -tiles (which corresponds to L and S , respectively) be $-1/\tau$ and 1, respectively, satisfying $r = -1/\tau$. Hence, A -tiles and B -tiles would be arranged as a Fibonacci lattice when we choose the strip width as $1 + 1/\tau = \tau$. We have considered a 1D arrangement of rectangle tiles (instead of pure 1D tiles of L and S) to encode the information of the embedded step into the string decoration. Now, the role of the strip is replaced by the height of the rectangles and, hence, is given by τ . The horizontal length of the tiles can have (fixed) finite, but any positive, values because we are interested in the sequence of A and B types, not the actual positions of vertices. The lengths in the pure 1D tiles of Fig. 3, $\cos\theta$ and $\sin\theta$, are chosen for the lifting to have a simple geometrical interpretation.

Although the mapping between the string decoration of our covering and the embedded step of Fibonacci tiling is simple, the physical implication of our growth algorithm is rather surprising. Contrary to conventional wisdom, it shows that a perfect 1D quasiperiodic structure can be grown with a pure local growth process. Debates on the possibility of a local growth algorithm for a quasiperiodic system has focused on 2D or 3D systems with the assumption that the local growth of a 1D quasiperiodic structure is impossible. Here, we have shown that the information on the whole sequence of A and B types can be encoded into the position of the string and passed to the attached new tile by a local process. In fact, this is the way that the long-range translational order is created in the crystal growth process. In crystal growth, a tile (unit-cell) joins to the existing patch of tiles side-by-side such that it fills the space without overlaps or gaps. By doing so, it carries information on the positions of all existing tiles; from its own position, we can calculate all possible positions of tiles compatible with its position although we do not know how many tiles already exist in the patch. The same information-transferring process happens in our quasicrystal growth process. From the position of string, we do not know how many tiles exist, but we can calculate all possible positions of the given types of tiles.

Previous local growth algorithms for the quasiperiodic structures [2, 11] are considered to be too complex for atoms to follow. Furthermore, they could produce only certain particular types of quasiperiodic structures with specially prepared seeds. The growth algorithm presented here is believed to apply for general quasiperiodic structures. By adjusting the decoration positions in the seeds, all classes of Fibonacci lattice structures [17] can be obtained. Furthermore, by changing the shapes of

the decorations and the heights of the tiles, we can grow all 1D quasiperiodic structures, which can be obtained by using the projection methods [19]. This new type of local growth algorithm may help us to answer the old puzzle of how quasicrystals grow with quasiperiodic order. Atomic structures of many quasicrystals, especially those that show high-quality quasiperiodic ordering, are well described by using quasi-unit-cell models [20, 21, 22] based on the covering with overlapping tiles. The overlap corresponds physically to the sharing of atoms by neighboring clusters. The overlaps are restricted to certain relative positions and orientations of the tiles according to overlap rules. Hence, it is a physically plausible assumption that decorations adjust their positions when they overlap with existing clusters of atoms. An important implication of this work is that atoms may relax their

positions in such a way that they carry long-range information on the atomic positions in other tiles and allow quasiperiodic structure to be grown by a local process. We hope that our observation can provide new insights as to how quasicrystals can grow in a structure with long-range quasiperiodic ordering.

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 - [13] Note that the three tiles (denoted by first three purple circles) at the left of site y must be in an *ABA* configuration regardless of the tile type at site y to avoid a *BB* or an *AAA* configuration in the twice inflated lattice, as illustrated by the blue double lines in Figs. 1(b) and (c).
 - [14] The length of a tile arrangement [patch, segments, etc.] are defined as the number of tiles in the arrangement [patch, segments]. We also define the range of a growth rule similarly. It is the number of tiles that are investigated to determine the type of the attaching tile.
 - [15] For $y_R < 1/\tau$, an *A*-tile is forced; otherwise, a *B*-tile is forced.
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